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SEARCH REQUEST FORM

Date: 12/2/99 Requester's Full Name: DAVID LUKTON Examiner #: 71263
Art Unit: 1654 Phone (308) 3213 Serial Number: 09/126958
Results Format Preferred (circle): PAPER DISK E-MAIL

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

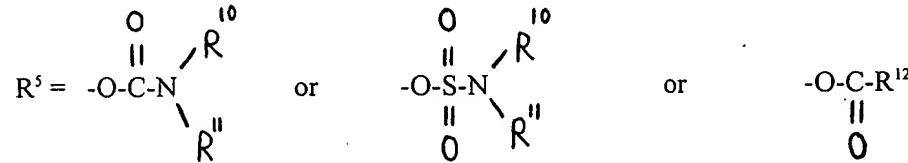
TITLE: CARBAMYLOXY COMPOUNDS WHICH INHIBIT LEUKOCYTE ADHESION
MEDIATED BY VLA-4

INVENTORS: (A) THORSETT,EUGENE D; (B) SEMKO,CHRISTOPHER M. (C)
SARANTAKIS, DIMITRIOS; (D) PLEISS,MICHAEL A. (E) KREFT,ANTHONY (F)
KONRADI, ANDREI W. (G) GRANT,FRANCINE S. (H) DRESSEN,DARREN B.; (I)
ASHWELL,SUSAN (J) BAUDY, REINHARDT BERNHARD (K) LOMBARDO,LOUIS JOHN

Priority Date: 7/31/97

Applicants are claiming the compounds on the attached sheet. The variables are as follows:

R¹ = anything;
R⁶ = anything;
R⁸ = anything;
R⁹ = anything;
Ar = aryl or heteroaryl;
n = 1 or 2;
x = 1 or 2;



wherein R¹⁰ and R¹¹ can be anything;
R¹² is any heterocyclic group;

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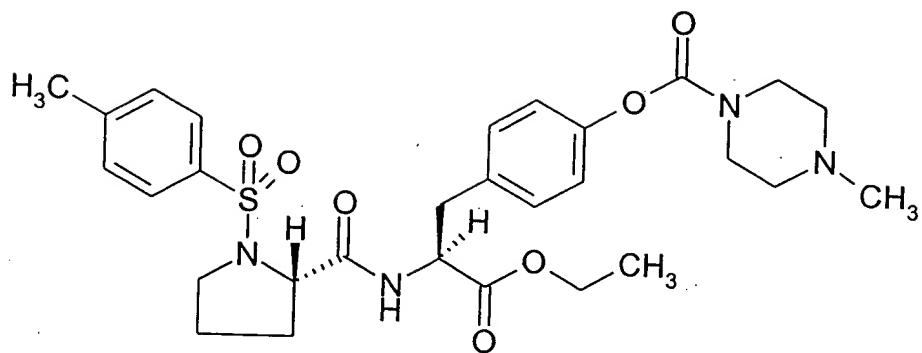
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Date Searcher Picked Up: _____
Date Completed: 12/8/99
Searcher Prep & Review Time: _____
Online Time: _____

Type of Search
NA Sequence (#) STN Dialog
AA Sequence (#) Questel/Orbit Dr. Link
Structure (#) Lexis/Nexis Westlaw
Bibliographic WWW/Internet
Litigation In-house sequence systems (list)
Fulltext Other (specify)
Other

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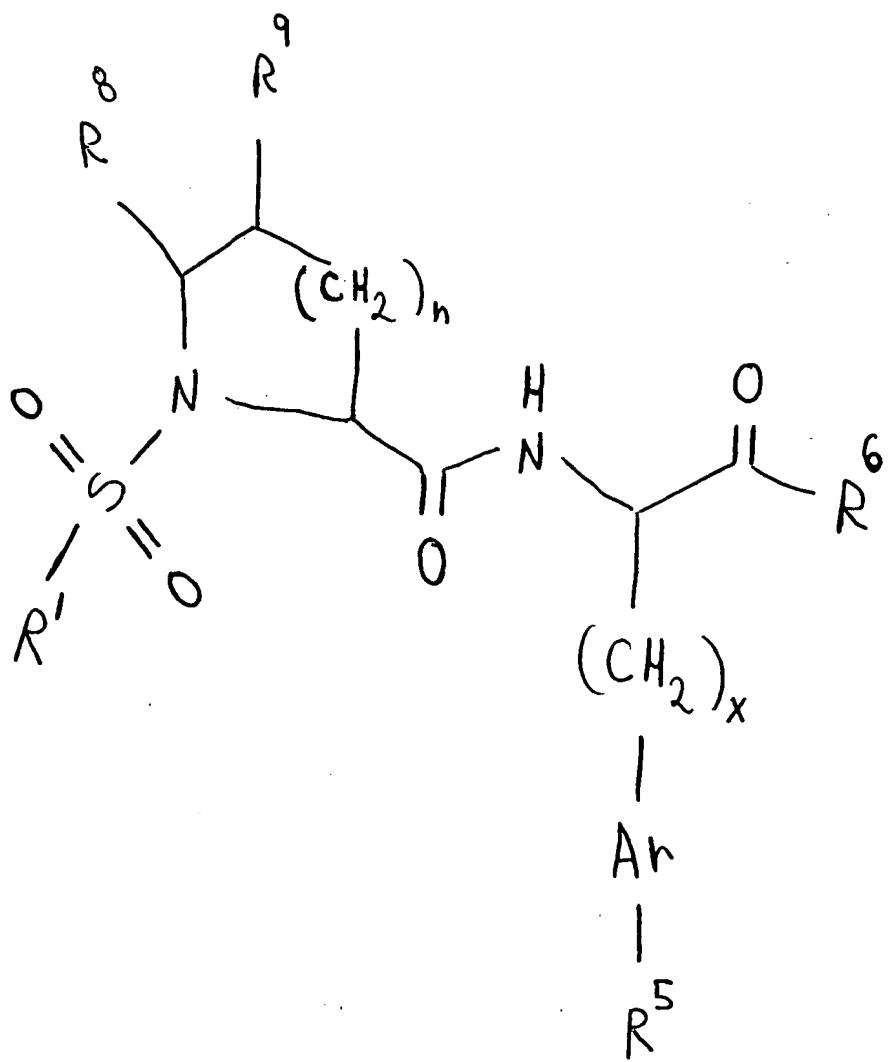
09/126, 958

Example of a claimed compound:



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09/126, 958



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=> fil hcplus

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FILE COVERS 1967 - 8 Dec 1999 VOL 131 ISS 24
 FILE LAST UPDATED: 7 Dec 1999 (19991207/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

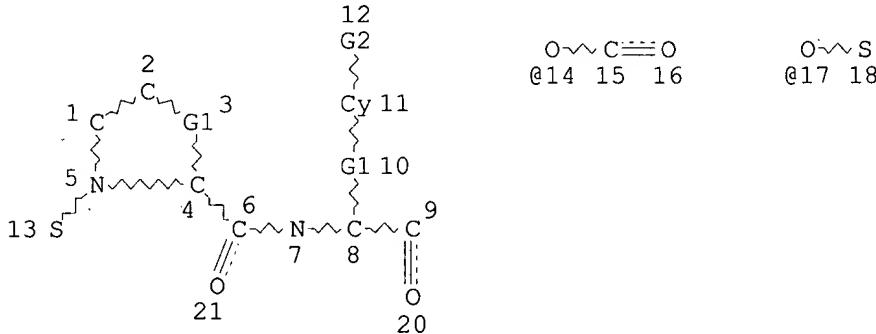
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L1 STR



REP G1=(0-1) C

VAR G2=14/17

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L3 214 SEA FILE=REGISTRY SSS FUL L1

L4 5 SEA FILE=HCPLUS ABB=ON PLU=ON L3

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L4 ANSWER 1 OF 5 HCPLUS COPYRIGHT 1999 ACS
 ACCESSION NUMBER: 1999:113712 HCPLUS
 DOCUMENT NUMBER: 130:168662
 TITLE: Preparation of N-sulfonylproline dipeptide derivatives and analogs as inhibitors of leukocyte adhesion mediated by VLA-4
 INVENTOR(S): Thorsett, Eugene D.; Semko, Christopher M.; Pleiss, Michael A.; Kreft, Anthony; Konradi, Andrei W.; Grant, Francine S.; Baudy, Reinhardt Bernhard; Sarantakis, Dimitrios
 PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; American Home Products Corporation
 SOURCE: PCT Int. Appl., 294 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906437	A1	19990211	WO 1998-US16070	19980731
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9888234	A1	19990222	AU 1998-88234	19980731
PRIORITY APPLN. INFO.:			US 1997-904423	19970731
			WO 1998-US16070	19980731

OTHER SOURCE(S): MARPAT 130:168662

AB Disclosed are title compds. R1SO2NR2CHR3QCHR5COR6 [R1 = (un)substituted alkyl, (un)substituted aryl, (un)substituted cycloalkyl, (un)substituted heterocyclyl; R2 = H, any group R1; R1R2 may form (un)substituted heterocyclic ring; R3 = H, any group R1; R2R3 may form (un)substituted heterocyclic ring; R5 = CH2X1; X1 = H, OH, acylamino, (un)substituted alkyl, alkoxy, aryloxy, aryl, aryloxyaryl, CO2H, carboxyalkyl, carboxyaryl, carboxyheteroaryl, (un)substituted cycloalkyl, (un)substituted heterocyclyl; Q = C(X)NR7; R7 = H, alkyl; X = O, S; R6 = NH2, (un)substituted alkoxy, (un)substituted cycloalkoxy, succinimidyl, adamantlyl, .beta.-cholest-5-en-3-yloxy, NHOY, NH(CH2)pCO2Y, OCH2NR9R10; Y = H, (un)substituted alkyl, (un)substituted aryl; p = 1-8; R9 = (un)substituted CO-aryl; R10 = H, CH2CO2R11, NHSO2Z'; R11 = alkyl; Z' = (un)substituted alkyl, (un)substituted cycloalkyl, (un)substituted aryl, (un)substituted heteroaryl, (un)substituted heterocyclyl; and pharmaceutically acceptable salts thereof, with provisos] which bind VLA-4 (also referred to as integrin .alpha.4.beta.1 and CD49d/CD29). Certain of these compds. also inhibit leukocyte adhesion and, in particular, leukocyte adhesion mediated by VLA-4. Such compds. are useful in the treatment of inflammatory diseases in a mammalian patient, e.g., human, wherein the disease may be, for example, asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, rheumatoid arthritis, tissue transplantation, tumor metastasis and myocardial ischemia. The compds. can also be administered for the treatment of inflammatory brain diseases such as multiple sclerosis. Thus, BOP-mediated peptide coupling of Ts-Pro-OH (Ts = tosyl) with H-Tyr-OMe gave 75% of the corresponding ester, which underwent sapon. in quant. yield to give desired dipeptide Ts-Pro-Tyr-OH. All prep'd. compds. have IC50 .1toreq. 15 .mu.M in a VLA-4 binding assay.

IT 220303-19-5P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(prepn. of N-sulfonylproline dipeptide derivs. and analogs as
inhibitors of leukocyte adhesion mediated by VLA-4)

L4 ANSWER 2 OF 5 HCPLUS COPYRIGHT 1999 ACS
 ACCESSION NUMBER: 1999:113710 HCPLUS
 DOCUMENT NUMBER: 130:153984
 TITLE: Preparation of N-sulfonyl dipeptide derivatives and
analogs as inhibitors of leukocyte adhesion mediated
by VLA-4
 INVENTOR(S): Thorsett, Eugene D.; Semko, Christopher M.; Pleiss,
Michael A.; Konradi, Andrei W.; Grant, Francine S.;
Dressen, Darren B.; Baudy, Reinhardt Bernhard
 PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; American Home
Products Corporation
 SOURCE: PCT Int. Appl., 151 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906435	A1	19990211	WO 1998-US15314	19980730
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9886612	A1	19990222	AU 1998-86612	19980730
PRIORITY APPLN. INFO.:			US 1997-904415	19970731
			WO 1998-US15314	19980730

OTHER SOURCE(S): MARPAT 130:153984

AB Disclosed are title compds. R1SO2NR2CR3R4QCHR5COR6 [R1 = (un)substituted alkyl, (un)substituted aryl, (un)substituted cycloalkyl, (un)substituted heterocycl; R2 = H, any group R1, (un)substituted cycloalkenyl; R1R2 may form heterocyclic ring; R3 = any group R1; R2R3 may form heterocyclic ring; R4 = any group R1; R3R4 may form cycloalkyl, (un)substituted heterocyclic ring; R5 = CHMe2, CH2X, :CHX1; X1 = H, OH, acylamino, optionally substituted alkyl, alkoxy, aryloxy, aryl, aryloxyaryl, carboxy, carboxyalkyl, etc.; Q = C(X)NR7, X = O, S, R7 = H, alkyl; X = O, S; R6 = NH2, (un)substituted alkoxy, (un)substituted cycloalkoxy, succinimidoxyl, adamantylamino, .beta.-cholest-5-en-3-yloxy, NHOY, NH(CH2)pCO2Y, OCH2NR9R10; Y = H, (un)substituted alkyl, (un)substituted aryl; p = 1-8; R9 = (un)substituted CO-aryl; R10 = H, CH2CO2R11, NHSO2Z; R11 = alkyl; Z = (un)substituted alkyl, (un)substituted cycloalkyl, (un)substituted aryl, (un)substituted heteroaryl, (un)substituted heterocycl; and pharmaceutically acceptable salts thereof, with provisos] which bind VLA-4 (also referred to as integrin .alpha.4.beta.1 and CD49d/CD29). Certain of these compds. also inhibit leukocyte adhesion and, in particular, leukocyte adhesion mediated by VLA-4. Such compds. are useful in the treatment of inflammatory diseases in a mammalian patient, e.g., human, wherein the disease may be, for example, asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, rheumatoid arthritis, tissue transplantation, tumor metastasis and myocardial ischemia. The compds. can also be administered for the treatment of inflammatory brain diseases such as multiple sclerosis. Thus, sulfonylation of cycloleucine (1-aminocyclopentanecarboxylic acid) with tosyl chloride, followed by peptide coupling with L-phenylalanine Me ester and sapon. gave desired title compd. 4-MeC6H4SO2-cycloleucyl-L-phenylalanine.

IT 220172-88-3P 220172-90-7P

RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of N-sulfonyl dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

IT 220172-89-4P 220172-92-9P 220173-39-7P
 220173-40-0P 220173-41-1P 220173-42-2P
 220173-43-3P 220173-45-5P 220173-47-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of N-sulfonyl dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

L4 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1999:113667 HCAPLUS
 DOCUMENT NUMBER: 130:177528
 TITLE: .alpha.9-Integrin antagonists and anti-inflammatory compositions
 INVENTOR(S): Yednock, Theodore A.; Pleiss, Michael A.
 PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA
 SOURCE: PCT Int. Appl., 60 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906391	A1	19990211	WO 1998-US15958	19980731
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9886050	A1	19990222	AU 1998-86050	19980731
EP 954519	A1	19991110	EP 1998-937310	19980731
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRIORITY APPLN. INFO.:			US 1997-904424	19970731
			US 1997-54453	19970801
			WO 1998-US15958	19980731

OTHER SOURCE(S): MARPAT 130:177528

AB Pharmaceutical compns. and methods are provided for treating inflammatory conditions, particularly those that are characterized by increased binding of .alpha.9-integrin to one or more of its ligands. Also disclosed are methods for selecting compds. for use in such compns. and methods.

IT 220543-91-9P 220543-92-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reaction; .alpha.9-integrin antagonists and anti-inflammatory compns.)

IT 220543-95-3 220543-99-7 220544-50-3

220545-11-9

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (.alpha.9-integrin antagonists and anti-inflammatory compns.)

IT 220543-93-1P 220543-94-2P 220605-30-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (.alpha.9-integrin antagonists and anti-inflammatory compns.)

L4 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1999:113666 HCAPLUS

DOCUMENT NUMBER: 130:182768
 TITLE: Preparation of N-sulfonyl O-carbamoyltyrosine dipeptide derivatives and analogs as inhibitors of leukocyte adhesion mediated by VLA-4
 INVENTOR(S): Thorsett, Eugene D.; Semko, Christopher M.; Sarantakis, Dimitrios; Pleiss, Michael A.; Kreft, Anthony; Konradi, Andrei W.; Grant, Francine S.; Dressen, Darren B.; Ashwell, Susan; Baudy, Reinhardt Bernhard; Lombardo, Louis John
 PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; American Home Products Corporation
 SOURCE: PCT Int. Appl., 386 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906390	A1	19990211	WO 1998-US15324	19980731
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9885849	A1	19990222	AU 1998-85849	19980731
PRIORITY APPLN. INFO.:			US 1997-904424	19970731
			US 1997-54453	19970801
			WO 1998-US15324	19980731

OTHER SOURCE(S): MARPAT 130:182768
 AB Disclosed are title compds. R1SO2NR2CHR3QCHR5COR6 [R1 = (un)substituted alkyl, (un)substituted aryl, (un)substituted cycloalkyl, (un)substituted heterocyclyl; R2 = H, any group R1; R1R2 may form (un)substituted heterocyclic ring; R3 = H, any group R1; R2R3 may form (un)substituted heterocyclic ring; R5 = (CH₂)_x-Ar-R5'; R5' = OZN8R8', OZR12; R8, R8' = independently H, (un)substituted alkyl, (un)substituted cycloalkyl, (un)substituted heterocyclyl; R12 = (un)substituted heterocyclyl; Z = CO, SO₂; Ar = (un)substituted aryl or heteroaryl; x = 1-4; Q = C(X)NR7; R7 = H, alkyl; X = O, S; R6 = NH₂, (un)substituted alkoxy, (un)substituted cycloalkoxy, succinimidyoxy, adamantlyl amino, .beta.-cholest-5-en-3-yloxy, NHOY, NH(CH₂)pCO₂Y, OCH₂NR9R10; Y = H, (un)substituted alkyl, (un)substituted aryl; p = 1-8; R9 = (un)substituted CO-aryl; R10 = H, CH₂CO₂R11, NHSO₂Z'; R11 = alkyl; Z' = (un)substituted alkyl, (un)substituted cycloalkyl, (un)substituted aryl, (un)substituted heteroaryl, (un)substituted heterocyclyl; and pharmaceutically acceptable salts thereof, with provisos] which bind VLA-4 (also referred to as integrin .alpha.4.beta.1 and CD49d/CD29). Certain of these compds. also inhibit leukocyte adhesion and, in particular, leukocyte adhesion mediated by VLA-4. Such compds. are useful in the treatment of inflammatory diseases in a mammalian patient, e.g., human, wherein the disease may be, for example, asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, rheumatoid arthritis, tissue transplantation, tumor metastasis and myocardial ischemia. The compds. can also be administered for the treatment of inflammatory brain diseases such as multiple sclerosis. Thus, carbamoylation of Ts-Pro-Tyr-OEt (Ts = tosyl) with Me₂NCOCl in the presence of Et₃N and DMAP gave 99% desired title compd. Ts-Pro-Tyr(CONMe₂)-OEt (I). Sapon. of I gave the corresponding free acid Ts-Pro-Tyr(CONMe₂)-OH. All prep'd. compds. have IC₅₀ > 10 μM in a VLA-4 binding assay.

IT 220543-91-9P 220543-92-0P 220543-99-7P
 220544-11-6P 220544-18-3P 220544-27-4P
 220544-46-7P 220544-48-9P 220544-64-9P

220544-65-0P 220544-66-1P 220544-67-2P
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220547-04-6P 220547-06-8P 220547-98-8P

RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
 study); PREP (Preparation); USES (Uses)

(prepn. of N-sulfonyl O-carbamoyltyrosine dipeptide derivs. and analogs
 as inhibitors of leukocyte adhesion mediated by VLA-4)

IT 220543-93-1P 220543-94-2P 220543-95-3P
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220551-46-2P 220551-47-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
 preparation); THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(prepn. of N-sulfonyl O-carbamoyltyrosine dipeptide derivs. and analogs
as inhibitors of leukocyte adhesion mediated by VLA-4)

IT 220548-09-4

RL: RCT (Reactant)

(prepn. of N-sulfonyl O-carbamoyltyrosine dipeptide derivs. and analogs
as inhibitors of leukocyte adhesion mediated by VLA-4)

L4 ANSWER 5 OF 5 HCPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1998:799992 HCPLUS

DOCUMENT NUMBER: 130:52724

TITLE: Preparation of heterocyclic dipeptide derivatives as
cell adhesion inhibitorsINVENTOR(S): Durette, Philippe L.; Hagmann, William K.; Maccoss,
Malcolm; Mills, Sander G.; Mumford, Richard A.; Van
Riper, Gail M.; Schmidt, Jack A.; Kevin, Nancy J.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

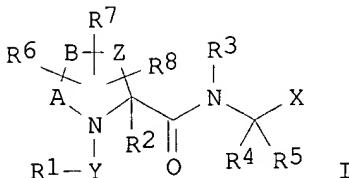
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9853814	A1	19981203	WO 1998-US10940	19980529
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			US 1997-48017	19970529
			GB 1997-14314	19970707
			US 1997-66525	19971125
			GB 1998-686	19980114

OTHER SOURCE(S): MARPAT 130:52724

GI



AB Title compds. I [R1 = (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, Cy, Cy-C1-10 alkyl, Cy-C2-10 alkenyl, Cy-C2-10 alkynyl; R2, R5 = independently (un)substituted H, C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, aryl, aryl-C1-10 alkyl, heteroaryl, heteroaryl-C1-10 alkyl; R3 = H, (un)substituted C1-10 alkyl, Cy, Cy-C1-10 alkyl; R4 = H, any group R1; R3R4 form mono- or bicyclic ring contg. 0-2 heteroatoms N, O, S; R4R5 form 3-7 membered mono- or bicyclic ring contg. 0-2 heteroatoms N, O, S; R10, R11 = independently = any group R3, (un)substituted C2-10 alkenyl, C2-10 alkynyl; R10R11 may form 5-7 membered heterocyclic ring contg. 0-2 addnl. heteroatoms N, O, S; R6-R8 = independently any group R10, OR10, NO2, halo, S(O)mR10, SR10, SO3R10, NR10R11, COR10, CO2R10, O2R10, CN, CONR10R11, CF3, oxo, NR10S(O)mR11, etc.; two of R6-R8 may form 5-7 membered (un)satd. monocyclic ring contg. 0-3 heteroatoms N, O, S; Cy = cycloalkyl, heterocyclyl, aryl, heteroaryl; A, Z = independently C, C-C; B = bond, C, C-C, N, O, S, S(O)m; X = CO2R10, P(O)(OR10)(OR11), P(O)(R10)(OR11), S(O)mOR10, CONR10R11, 5-tetrazolyl; Y = CO, O2C, NR11CO, SO2, P(O)(OR4), COCO; m = 1-2] = are antagonists of VLA-4 and/or .alpha.4.beta.7, and are useful for inhibition or prevention of cell adhesion and cell adhesion

mediated pathologies. These compds. may be formulated into pharmaceutical compns. and are suitable for use in the treatment of asthma, allergies, inflammation, multiple sclerosis, and other inflammatory and autoimmune disorders. Thus, coupling of L-2-naphthylalanine tert-Bu ester (H-Nal-OtBu) (prepn. given) with Cbz-Pro-OH (Cbz = PhCH₂O₂C), followed by catalytic deprotection, sulfonylation with 3,5-C₁₂C₆H₃SO₂Cl, and acidic deesterification gave desired N-sulfonyldipeptide C₁₂C₆H₃SO₂-Nal-Pro-OH. Procedures for inhibition of VLA-4 dependent adhesion to a CS-1 conjugate and VCAM-IG fusion protein are given.

IT
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 217453-30-0P 217453-31-1P 217453-32-2P
 217453-33-3P 217453-34-4P 217453-35-5P
 217453-36-6P 217453-37-7P 217453-38-8P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of heterocyclic dipeptide derivs. as cell adhesion inhibitors)

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=> fil caold

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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 DICTIONARY FILE UPDATES: 07 DEC 99 HIGHEST RN 250252-89-2

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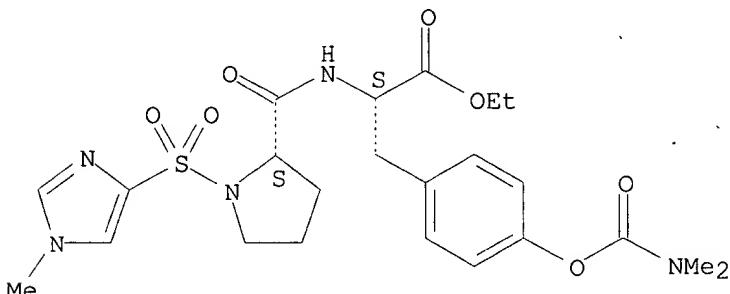
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Absolute stereochemistry.

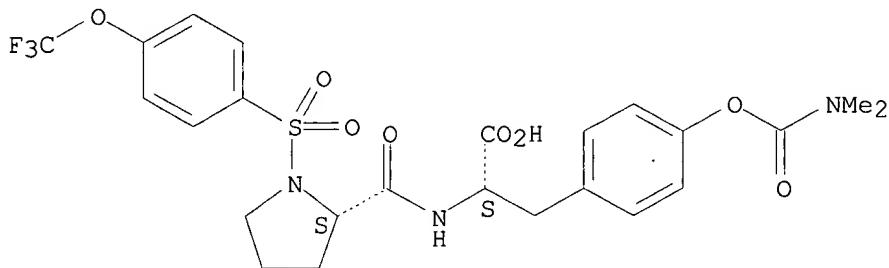


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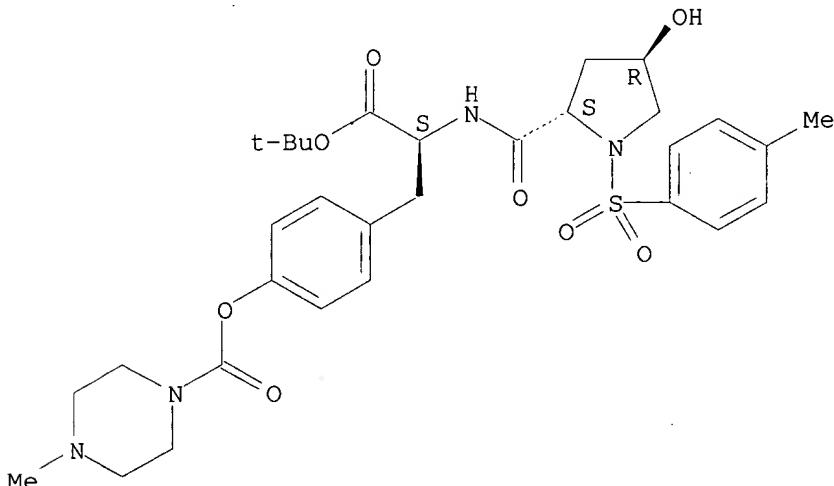


1 REFERENCES IN FILE CA (1967 TO DATE)
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REFERENCE 1: 130:182768

L3 ANSWER 4 OF 214 REGISTRY COPYRIGHT 1999 ACS
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Absolute stereochemistry.

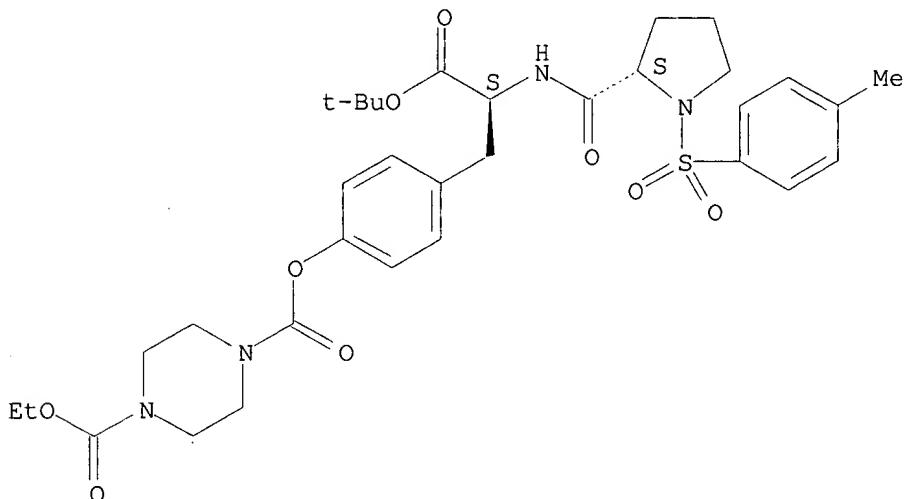


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REFERENCE 1: 130:182768

L3 ANSWER 6 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220547-99-9 REGISTRY
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Absolute stereochemistry.

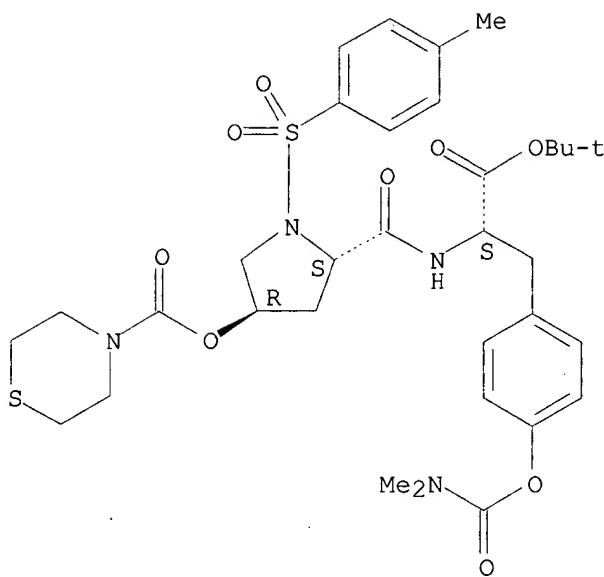


1 REFERENCES IN FILE CA (1967 TO DATE)
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REFERENCE 1: 130:182768

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Absolute stereochemistry.

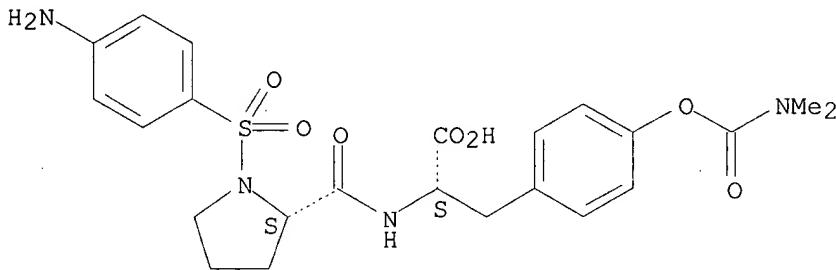


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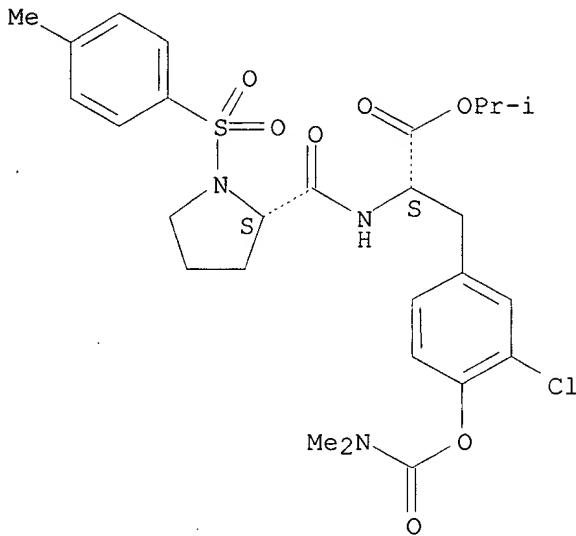


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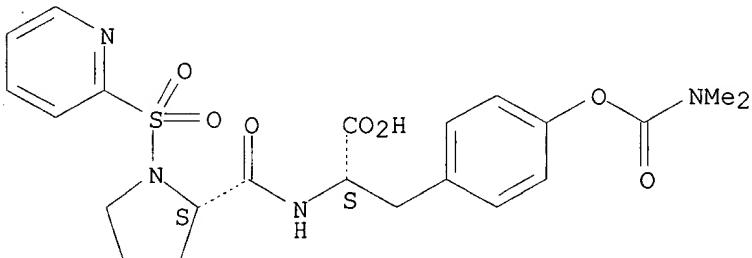


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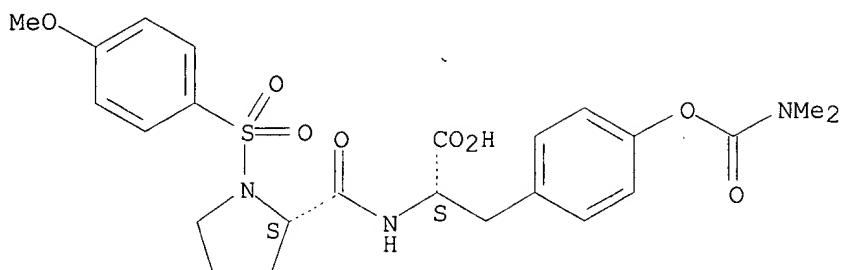


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Absolute stereochemistry.

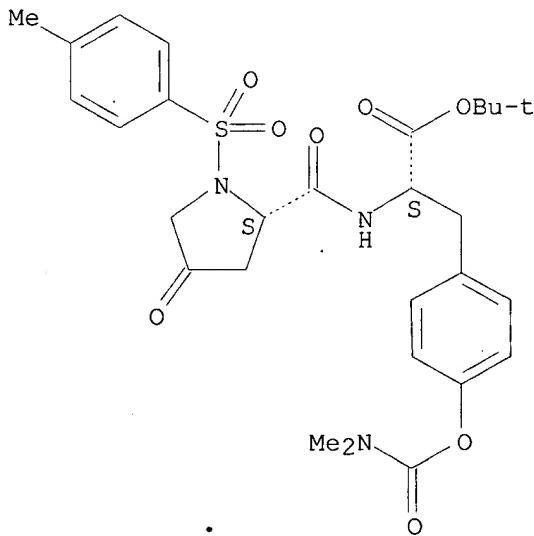


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Absolute stereochemistry.



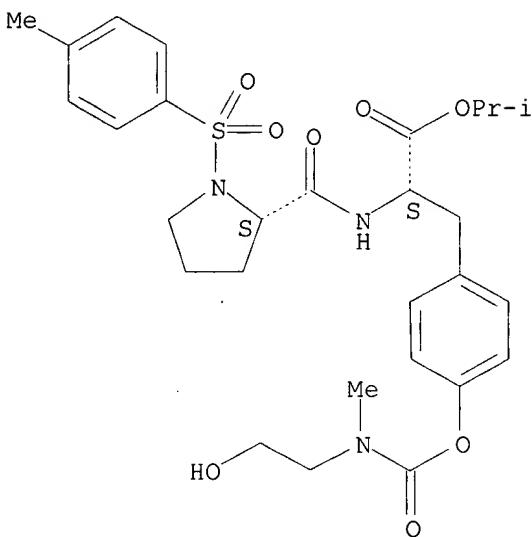
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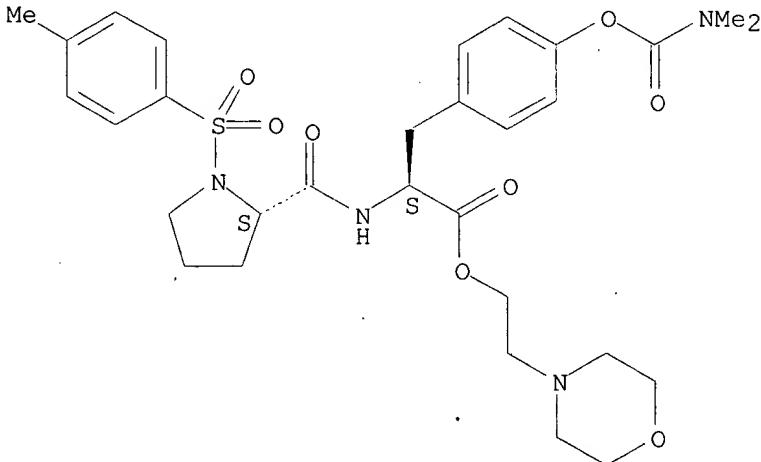


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 110 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220545-34-6 REGISTRY
 CN L-Tyrosine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-, 2-(4-morpholinyl)ethyl ester, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C30 H40 N4 O8 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

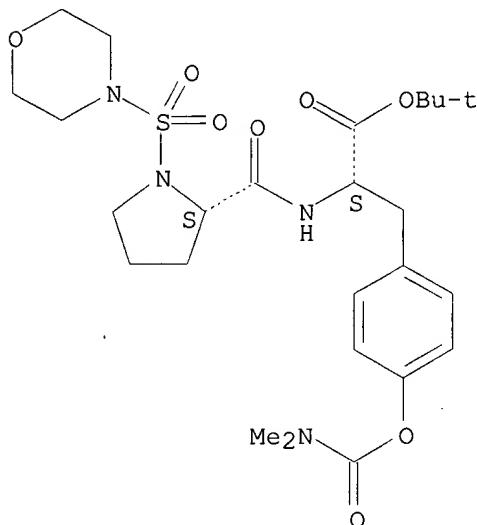


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 120 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220545-22-2 REGISTRY
 CN L-Tyrosine, 1-(4-morpholinylsulfonyl)-L-prolyl-, 1,1-dimethylethyl ester,
 dimethylcarbamate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H38 N4 O8 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

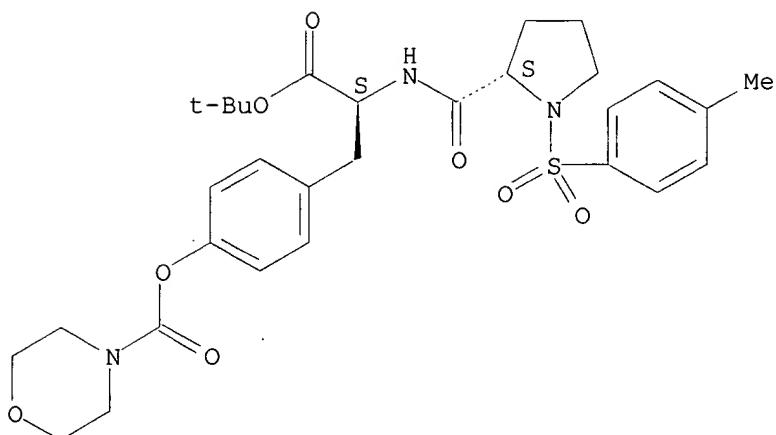


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 138 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220544-94-5 REGISTRY
 CN L-Tyrosine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-, 1,1-dimethylethyl
 ester, 4-morpholinecarboxylate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C30 H39 N3 O8 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

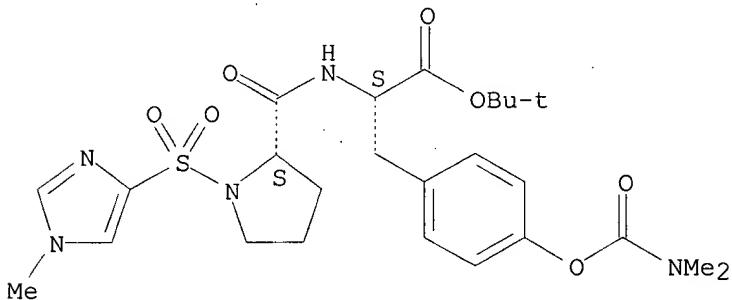


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 140 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220544-90-1 REGISTRY
 CN L-Tyrosine, 1-[(1-methyl-1H-imidazol-4-yl)sulfonyl]-L-prolyl-,
 1,1-dimethylethyl ester, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H35 N5 O7 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

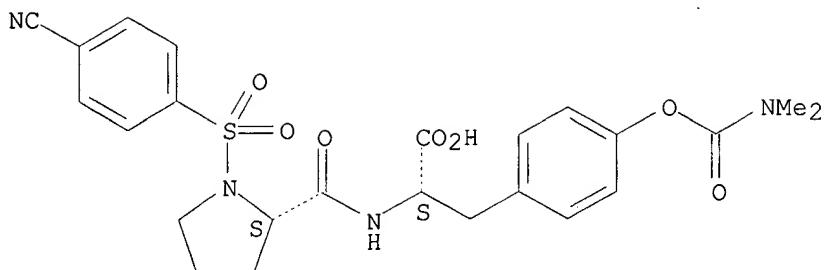


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 150 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220544-79-6 REGISTRY
 CN L-Tyrosine, 1-[(4-cyanophenyl)sulfonyl]-L-prolyl-, dimethylcarbamate
 (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C24 H26 N4 O7 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

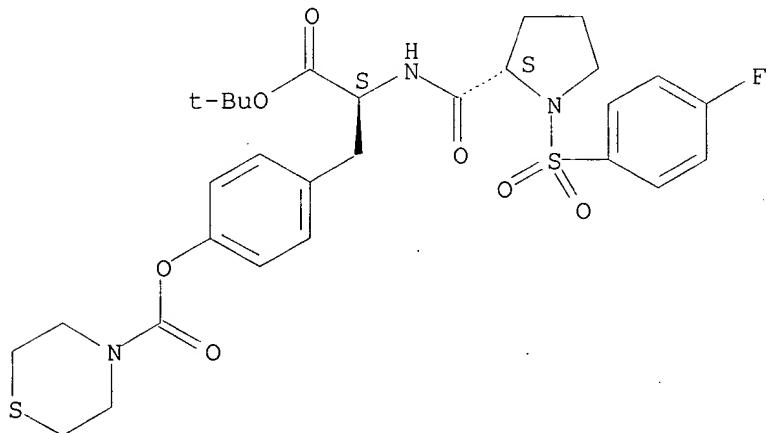


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 160 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220544-55-8 REGISTRY
 CN L-Tyrosine, 1-[(4-fluorophenyl)sulfonyl]-L-prolyl-, 1,1-dimethylethyl ester, 4-thiomorpholinecarboxylate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C29 H36 F N3 O7 S2
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

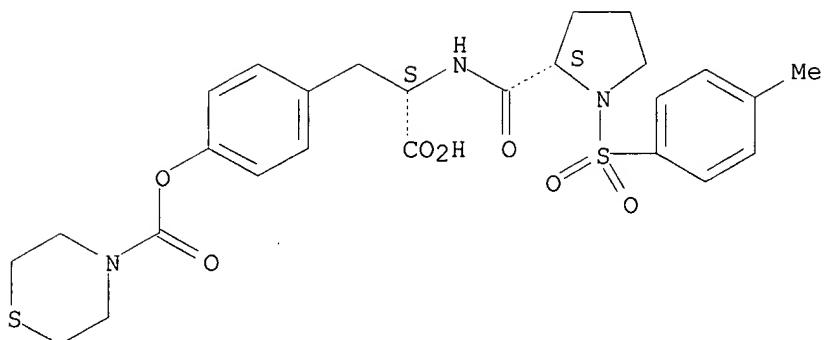


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 170 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220544-32-1 REGISTRY
 CN L-Tyrosine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-, 4-thiomorpholinecarboxylate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C26 H31 N3 O7 S2
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

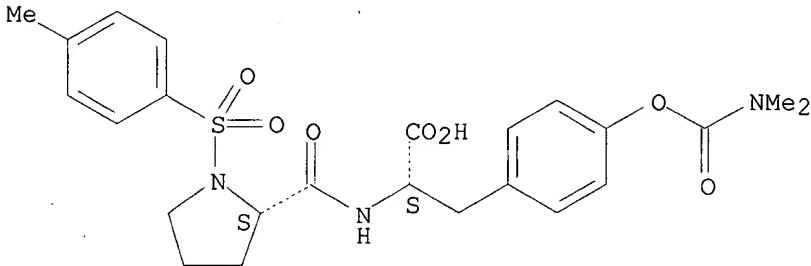


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

L3 ANSWER 179 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220543-99-7 REGISTRY
 CN L-Tyrosine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-, dimethylcarbamate
 (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C24 H29 N3 O7 S
 SR CA
 LC STN Files: CA, CAPLUS, TOXLIT

Absolute stereochemistry.



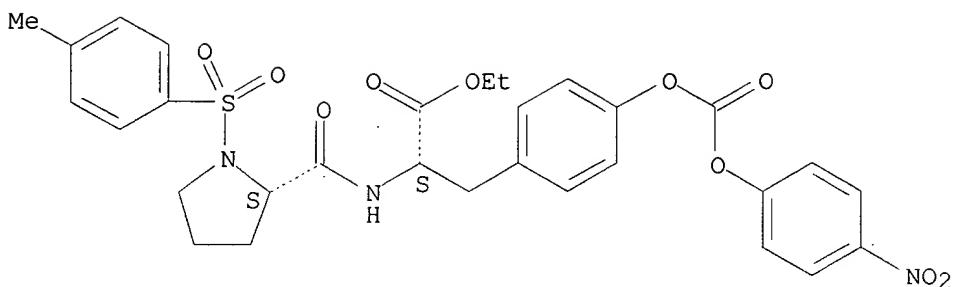
2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:182768

REFERENCE 2: 130:177528

L3 ANSWER 188 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220303-19-5 REGISTRY
 CN L-Tyrosine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-, ethyl ester,
 4-nitrophenyl carbonate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C30 H31 N3 O10 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

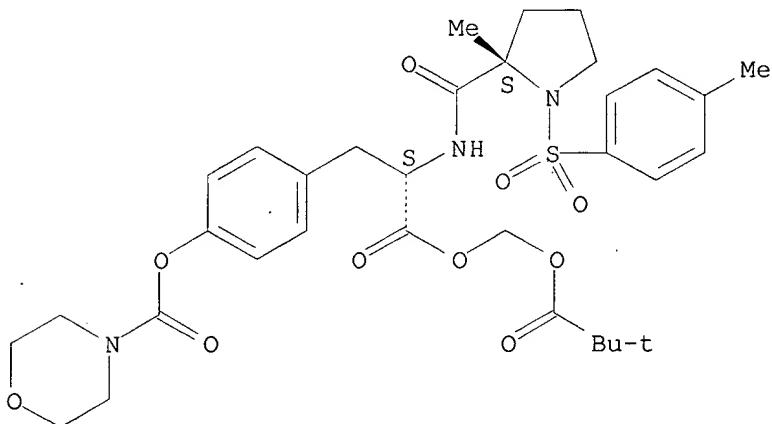


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:168662

L3 ANSWER 189 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220173-47-7 REGISTRY
 CN L-Tyrosine, 2-methyl-1-[(4-methylphenyl)sulfonyl]-L-prolyl-,
 (2,2-dimethyl-1-oxoproxy)methyl ester, 4-morpholinecarboxylate (ester)
 (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C33 H43 N3 O10 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

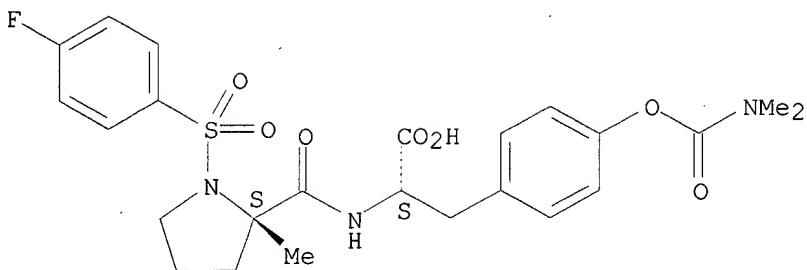


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:153984

L3 ANSWER 196 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 220172-92-9 REGISTRY
 CN L-Tyrosine, 1-[(4-fluorophenyl)sulfonyl]-2-methyl-L-prolyl-,
 dimethylcarbamate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C24 H28 F N3 O7 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

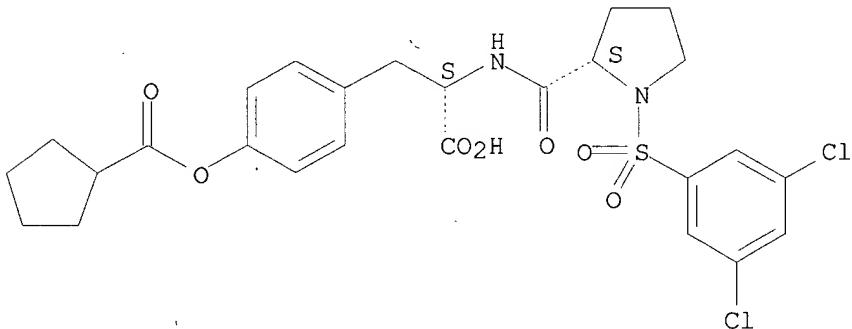


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:153984

L3 ANSWER 200 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 217453-38-8 REGISTRY
 CN L-Tyrosine, 1-[(3,5-dichlorophenyl)sulfonyl]-L-prolyl-,
 cyclopentanecarboxylate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C26 H28 Cl2 N2 O7 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

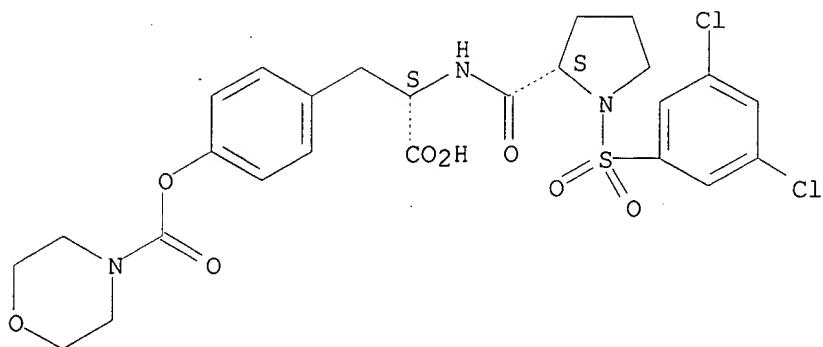


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:52724

L3 ANSWER 210 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 217453-22-0 REGISTRY
 CN L-Tyrosine, 1-[(3,5-dichlorophenyl)sulfonyl]-L-prolyl-,
 4-morpholinocarboxylate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H27 Cl2 N3 O8 S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

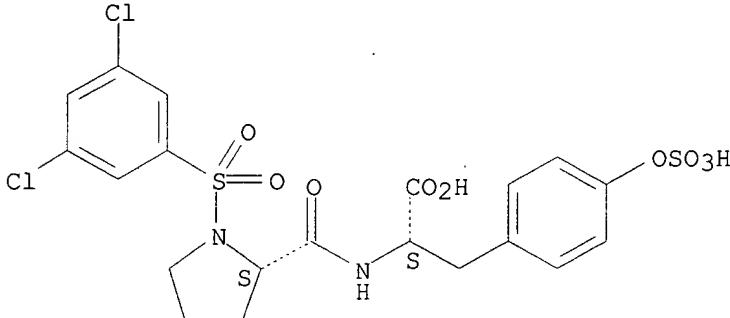


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:52724

L3 ANSWER 214 OF 214 REGISTRY COPYRIGHT 1999 ACS
 RN 217450-85-6 REGISTRY
 CN L-Tyrosine, 1-[(3,5-dichlorophenyl)sulfonyl]-L-prolyl-, hydrogen sulfate (ester) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C20 H20 Cl2 N2 O9 S2
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:52724